Microscopic Spectrum of the Wilson Dirac Operator

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We calculate the leading contribution to the spectral density of the Wilson Dirac operator using chiral perturbation theory where volume and lattice spacing corrections are given by universal scaling functions. We find analytical expressions for the spectral density on the scale of the average level spacing, and introduce a chiral Random Matrix Theory that reproduces these results. Our work opens up a novel approach to the infinite volume limit of lattice gauge theory at finite lattice spacing and new ways to extract coefficients of Wilson chiral perturbation theory.

Introduction. Spectral gaps and their suppression by disorder are essential for a variety of physical phenomena. States that intrude into the band gap, so called Lifshitz tail states, affect the conductivity of semiconductors [1], they may lead to gapless superconductivity in superconductors with magnetic impurities [2], and they may show universal fluctuations given by Random Matrix Theory (see [3]). Here we analyze the spectrum of the Wilson Dirac operator of lattice Quantum Chromodynamics (QCD). In the continuum limit, the Hermitian Wilson Dirac operator has a gap equal to twice the quark mass. At finite lattice spacing, eigenvalues of tail states intrude into the gap. When eigenvalues approach the center of the gap, it becomes increasingly difficult to invert the Wilson Dirac operator. As a consequence, such tail states can potentially obstruct lattice simulations. It is therefore of importance to have an analytical understanding of the properties of these states.

Our results rely on two approaches, chiral Random Matrix Theory and chiral Lagrangians for the pseudo-Nambu-Goldstone sector of QCD. The relation between chiral Random Matrix Theory and the Dirac operator in theories with spontaneously broken chiral symmetries [4] has led to a new understanding of the chiral limit of strongly coupled gauge theories. The Random Matrix Theory results are universal [5] and are equivalent [6] to what is obtained from a chiral Lagrangian in the microscopic domain or ϵ -regime [7]. This gives a finitevolume scaling theory for spectral correlation functions as well as individual eigenvalue distributions of the continuum Dirac operator at fixed topological charge ν . In lattice QCD it has become standard to utilize these results to obtain physical observables from simulations at finite four-volume V. There has for long been a desire to obtain analogous results for Wilson fermions at finite lattice spacing a. Here we present a solution to this problem.

We denote the Wilson Dirac operator by $D = D_W + m$.

Below we make use only of its block structure given by

$$D_W = \begin{pmatrix} aA & W \\ -W^{\dagger} & aB \end{pmatrix} \tag{1}$$

with $A^{\dagger}=A$ and $B^{\dagger}=B$, whereas W does not have additional symmetry properties. The Wilson Dirac operator is anti-Hermitian in the continuum limit $a \to 0$ and the corresponding eigenvalues of D_W are complex away from the continuum limit.

Although non-Hermitian, the Wilson Dirac operator satisfies γ_5 -Hermiticity

$$D^{\dagger} = \gamma_5 D \gamma_5 \ . \tag{2}$$

Instead of the Wilson Dirac operator itself, it is therefore often more convenient to work with the Hermitian Dirac operator $D_5 = \gamma_5 D$. At zero lattice spacing, the spectrum of D_5 has a gap around the origin of width 2m. At non-zero lattice spacing a, states intrude inside the gap and for sufficiently large lattice spacing the gap closes. Then one enters what is known as the Aoki phase [8]. It is reminiscent of the Gorkov Hamiltonian for superconductors, where magnetic impurities (see [2, 3]) play the role of the diagonal blocks in Eq. (1) and the Aoki phase corresponds to gapless superconductivity. A first order scenario where the condensate jumps as a function of m has been suggested [9] and support for this has been found on the lattice [10].

The spectral density $\rho_5(x)$ of D_5 , evaluated at x=0, is an order parameter [11] for the onset of the Aoki phase. Discretization effects in the spectrum of the Wilson Dirac operator were analyzed by means of chiral perturbation theory in [12]. What is new here is that we obtain an exact analytical description in the microscopic scaling limit and show in detail the transition to the Aoki phase. This opens a novel analytical approach to the infinite-volume limit of lattice gauge theory at finite lattice spacing and offers new ways to measure the leading coefficients of Wilson chiral perturbation theory. Understanding the distributions of the low-lying eigenvalues of the Wilson Dirac operator is also crucial for establishing a stable domain for numerical simulations [13].

Chiral Lagrangian. The leading-order terms of the chiral Lagrangian for Wilson fermions have been listed in [9]. It is a double expansion: the continuum ordering for chiral perturbation theory and an expansion in the lattice spacing a. The corresponding chiral Lagrangian coincides with the continuum Lagrangian with shifted mass plus terms starting at order a^2 . It is convenient to introduce a source for $\bar{\psi}\gamma_5\psi$, which we denote by z. Here, we shall focus on the microscopic domain where mV, zVand a^2V are kept fixed in the infinite-volume limit. Different counting rules are possible [14], but the present one is most useful for elucidating the effects of finite lattice spacing on the low-lying Dirac eigenvalues. The leading contribution to the finite-volume QCD partition function then reduces to a unitary matrix integral, which, up to a few constants, is determined by symmetry arguments. We decompose this partition function as $Z_{N_f} = \sum_{\nu} Z_{N_f}^{\nu}$ with

$$Z_{N_f}^{\nu}(m,z;a) = \int_{U(N_f)} dU \, \det^{\nu} U \, e^{S[U]}$$
 (3)

where the action S[U] for degenerate quark masses is

$$S = \frac{m}{2} \Sigma V \text{Tr}(U + U^{\dagger}) + \frac{z}{2} \Sigma V \text{Tr}(U - U^{\dagger})$$

$$-a^{2} V W_{6} [\text{Tr} (U + U^{\dagger})]^{2} - a^{2} V W_{7} [\text{Tr} (U - U^{\dagger})]^{2}$$

$$-a^{2} V W_{8} \text{Tr}(U^{2} + U^{\dagger^{2}}).$$

$$(4)$$

Below we will demonstrate that in the microscopic domain $Z_{N_f}^{\nu}$ corresponds to ensembles of gauge field configurations with ν real modes of D_W . The a^2 -terms are determined by invariance arguments [9], and Σ , W_6 , W_7 and W_8 are the low-energy constants of $\mathcal{O}(a^2)$ Wilson ChPT. The two terms corresponding to W_6 and W_7 are expected to be suppressed in the large- N_c limit [15], and we shall for simplicity ignore them here. The potential impact of these terms [16] can be studied at the expense of a slightly more cumbersome analysis. The leading finite-volume partition function $Z_{N_f}^{\nu}$ then only depends on the microscopic scaling variables $\hat{m} = m\Sigma V$, $\hat{z} = z\Sigma V$, and $\hat{a} = a\sqrt{W_8V}$ which will be kept fixed for $V \to \infty$. The sign of W_8 will be discussed below.

The Generating Function. A generating function for spectral correlation functions is given by an average of ratios of determinants. Because of the inverse determinants, it has an extended graded flavor symmetry. The graded generating function for spectral correlations of D_5 is

$$Z_{k|l}^{\nu}(\mathcal{M}, \mathcal{Z}; \hat{a}) = \int dU \operatorname{Sdet}(U)^{\nu}$$

$$(5)$$

$$\underset{\mathcal{L}}{\vee} e^{i\frac{1}{2}\operatorname{Str}(\mathcal{M}[U-U^{-1}]) + i\frac{1}{2}\operatorname{Str}(\mathcal{Z}[U+U^{-1}]) + \hat{a}^{2}\operatorname{Str}(U^{2}+U^{-2})}$$

where $\mathcal{M} \equiv \operatorname{diag}(\hat{m}_1 \dots \hat{m}_{k+l})$ and $\mathcal{Z} \equiv \operatorname{diag}(\hat{z}_1 \dots \hat{z}_{k+l})$. This graded partition function differs in a subtle way from the one introduced in [12]. As discussed in [6], the

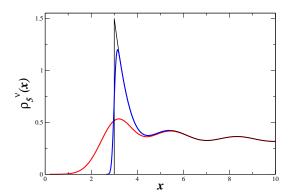


FIG. 1: The microscopic spectrum of D_5 for $\hat{m}=3, \nu=0$ and $\hat{a}=0, 0.03,$ and 0.250. The $\nu=0$ spectrum is reflection symmetric about $\hat{x}=0$.

integration manifold for non-perturbative computations is non-compact for the bosonic sector. While the action (5) and the action introduced in [12] break the flavor symmetries in exactly the same way, only the former one is consistent with the convergence requirements of the graded integral for $W_8 > 0$. For perturbative calculations the convergence requirements are immaterial. Here and below we focus mainly on the quenched case, corresponding to integration manifold Gl(1|1)/U(1). The generalization to an arbitrary number of flavors is straightforward, and we expect that the underlying integrability structure will lead to a full analytical solution just as in the a=0 case [17].

The Microscopic Spectrum of D_5 . For a=0, the microscopic spectral density of D_5 follows from the expression for the microscopic spectral density of D through

$$\rho_5^{\nu}(\hat{x} > \hat{m}, \hat{m}; \hat{a} = 0) = \frac{\hat{x}}{\sqrt{\hat{x}^2 - \hat{m}^2}} \rho^{\nu} (\sqrt{\hat{x}^2 - \hat{m}^2}) . \quad (6)$$

To obtain the spectral density of D_5 for $a \neq 0$, we evaluate the resolvent

$$G^{\nu}(\hat{z}, \hat{m}; \hat{a}) \equiv \lim_{\hat{z}' \to \hat{z}} \frac{d}{d\hat{z}} Z^{\nu}_{1|1}(\hat{m}, \hat{m}, \hat{z}, \hat{z}'; \hat{a})$$
 (7)

and find

$$G^{\nu}(\hat{z}, \hat{m}; \hat{a}) = \int_{-\infty}^{\infty} ds \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \frac{i}{2} \cos(\theta) e^{S_f + S_b} e^{(i\theta - s)\nu} \times (-\hat{m}\sin(\theta) + i\hat{m}\sinh(s) + i\hat{z}\cos(\theta) + i\hat{z}\cosh(s)$$
(8)
+4\hat{a}^2[\cos(2\theta) + \cosh(2s) + (e^{i\theta + s} + e^{-i\theta - s})] + 1).

Here $S_f = -\hat{m}\sin(\theta) + i\hat{z}\cos(\theta) + 2\hat{a}^2\cos(2\theta)$ and $S_b = -i\hat{m}\sinh(s) - i\hat{z}\cosh(s) - 2\hat{a}^2\cosh(2s)$. As is well known, the resolvent is defined only up to ultraviolet subtractions in the underlying theory. The microscopic quenched spectral density,

$$\rho_5^{\nu}(\hat{x}, \hat{m}; \hat{a}) = \frac{1}{\pi} \text{Im}[G^{\nu}(\hat{x}, \hat{m}; \hat{a}))], \tag{9}$$

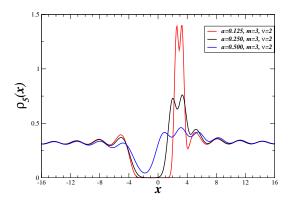


FIG. 2: The microscopic spectrum of D_5 for $\hat{m} = 3$, $\nu = 2$ and $\hat{a} = 0.125$, $\hat{a} = 0.250$ and $\hat{a} = 0.500$ respectively.

is, however, uncontaminated by these ultraviolet pieces. Plots of ρ_5^{ν} are shown in Fig. 1 for $\nu = 0$, and in Fig. 2 for $\nu = 2$. The eigenvalues that converge towards the endpoints of the spectrum at $sign(\nu)m$ in the $a\to 0$ limit are clearly visible. The sum over ν of the spectral density, for which the continuum limit has been established rigorously [18], can be evaluated in a straightforward way. Random Matrix Theory. An efficient alternative way to extend the above results to all spectral correlation functions and individual eigenvalue distributions is to construct a chiral Random Matrix Theory that is equivalent to the chiral Lagrangian in the same scaling regime. This the case if the chiral Random Matrix Theory has the same global symmetries and transformation properties as the QCD partition function with the Wilson Dirac operator. The chiral Random Matrix Theory is

$$\tilde{Z}_{N_f}^{\nu} = \int d\tilde{A}d\tilde{B}d\tilde{W} \det^{N_f}(\tilde{D}_W + \tilde{m} + \tilde{z}\tilde{\gamma}_5) P(\tilde{D}_W), (10)$$

where \hat{D}_W is of the same block form as (1) and the integration is over the real and imaginary parts of the matrix elements of the Hermitian $n \times n$ matrix, A, the Hermitian $(n+\nu)\times(n+\nu)$ matrix \tilde{B} and the complex $n\times(n+\nu)$ matrix \tilde{W} . This \tilde{D}_W has $|\nu|$ real eigenvalues. We have added tildes to stress that this is a zero-dimensional matrix integral with parameters \tilde{m} and \tilde{z} instead of m and z. In the universal scaling limit there is a one-to-one correspondence between the two pairs, just as in the a=0case. The precise form of the distribution of the matrix elements $P(\tilde{D}_W)$ is not important on account of universality. The partition function (3) (with $W_6 = W_7 = 0$) is recovered in the microscopic scaling limit. For a Gaussian distribution, this can be shown by a simple explicit calculation. It also follows that $W_8 > 0$. This is a consequence of the γ_5 -Hermiticity: Changing the sign of W_8 is equivalent to $a \to ia$, violating γ_5 -Hermiticity of \tilde{D}_W . This suggests that the Hermiticity properties of the Dirac operator can restrict the coefficients of the effective Lagrangian. In fact, with $W_8 < 0$ the integrals in (5) are

divergent. However, the graded partition function

$$\bar{Z}_{1|1}^{\nu}(\mathcal{M}, \mathcal{Z}; \hat{a}) = \int dU \operatorname{Sdet}(U)^{\nu}$$

$$\times e^{\frac{1}{2}\operatorname{Str}(\mathcal{M}[U+U^{-1}]) + \frac{1}{2}\operatorname{Str}(\mathcal{Z}[U-U^{-1}]) - \hat{a}^{2}\operatorname{Str}(U^{2} + U^{-2})}$$
(11)

is now convergent. Repeating the steps leading to (7) with this convergent integral, we find a resolvent for an operator that, unlike D_5 , is not Hermitian. We believe that the absence of solutions in the p-regime [12] for $W_8 < 0$ has the same origin.

The ensemble with the structure of the matrix \tilde{D}_W belongs to one of the classes in the non-Hermitian classification of [19] (the γ_5 -Hermiticity is there referred to as Q-symmetry). In the microscopic scaling limit, the partition function (10) has the determinantal structure

$$Z_{N_f}^{\nu}(\hat{m}, \hat{z}; \hat{a}) = \det[Z_{N_f=1}^{\nu+i-j}(\hat{m}, \hat{z}; \hat{a})]_{i,j=1...N_f}$$
 (12)

where

$$Z_1^{\nu} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i\theta\nu} e^{\hat{m}\cos(\theta) + i\hat{z}\sin(\theta) - 2\hat{a}^2\cos(2\theta)}.$$
 (13)

This form suggests that the partition function is a τ -function of an integrable system of Toda type and that an eigenvalue representation can be obtained.

The simplest quantity to compute from (12) is the chiral condensate, $\Sigma(\hat{m}) = \partial_{\hat{m}} \log Z$. For $\nu = 0$ there is a striking similarity to the chiral condensate for QCD at non-zero isospin chemical potential μ . The condensate is constant for large \hat{m} and drops roughly linearly to zero inside a well defined region (the Aoki phase and the pion condensed phase, respectively). This is not accidental: The microscopic spectrum of D_W at $a \neq 0$ forms a thin strip along the imaginary axis just as the continuum Dirac operator does at $\mu \neq 0$. In both cases, the chiral condensate can be interpreted as the electric field at m of point charges at the position of the eigenvalues. Also the convergence requirements of the graded partition function (5) have direct analogues at nonzero chemical potential [20].

The Density of Real Modes. The analytical result for the quenched average spectral density of the real eigenvalues, denoted by $\rho_{\text{Wreal}}^{\nu}$, also follows from the generating function (5) (a derivation will be given in [21]). A plot of $\rho_{\text{Wreal}}^{\nu}$ for $\nu=4$ versus $\hat{\zeta}\equiv\zeta\Sigma V$ is shown in Fig. 3. The real eigenvalues, ζ_i , of D_W repel each other and the $|\nu|=4$ real modes are clearly visible. We have checked that the distribution is in agreement with the chiral Random Matrix Theory (10). This illustrates that in the label ν introduced in (3) corresponds to the number of real eigenvalues. For large ν we find that $\rho_{\text{Wreal}}^{\nu}$ approaches a semi-circle. We suggest that analyzing just these real eigenmodes of D_W may provide a new useful tool in lattice QCD.

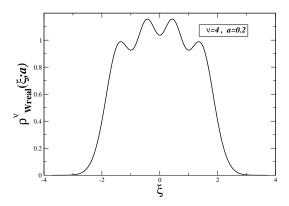


FIG. 3: The quenched density of the real eigenvalues of D_W .

Distribution of Tail States. For $|\hat{x} - \hat{m}|/\hat{a}^2 \gg 1$ and $8\hat{a}^2 \ll 1$ the tail of the spectral density inside the gap follows from a saddle point analysis. For $\hat{x} > 0$ we find

$$\rho_5(\hat{x}) \sim \exp[-(\hat{x} - \hat{m})^2 / 16\hat{a}^2],$$
 (14)

and a similar result for $\hat{x} < 0$. This result applies to the tail of the blue and (marginally) of the red curve in Fig. 1. Reinstating physical parameters we find that the width parameter, σ , in (14) is given by $\sigma^2 = 8a^2W_8/(V\Sigma^2)$ so that, in the microscopic domain and sufficiently small \hat{a} , σ scales with $1/\sqrt{V}$. Such a scaling has been observed for $N_f = 2$ in [13, 22].

Tail states may also be studied in their own right and for applications in condensed matter physics. In particular, in the thermodynamic limit, $\hat{m}, \hat{x}, \hat{a}^2 \gg 1$, the average level density of D_5 can be obtained by a saddle point analysis. For $8\hat{a}^2/\hat{m} < 1$ it vanishes inside $[-\hat{x}_c, \hat{x}_c]$ with \hat{x}_c given by $\hat{x}_c = 8\hat{a}^2 \left[(\hat{m}/8\hat{a}^2)^{2/3} - 1 \right]^{3/2}$. It has exactly the same form as for superconductors with magnetic impurities [2]. In the scaling limit where $V^{2/3}(x_c - x)$ is kept fixed, the spectral density can be computed inside the gap by a saddle point approximation of (5), and it agrees with universal Random Matrix Theory results for the so-called soft edge. Such universal behaviour has also been found in condensed matter systems [2, 3].

Conclusions. Using a graded chiral Lagrangian for Wilson fermions at finite lattice spacings, we have obtained an analytical form for the Wilson Dirac spectrum at fixed number, ν , of real eigenvalues. These results, and their extensions to dynamical fermions, should be useful for lattice simulations at finite volume. We have shown how the leading low-energy constant for Wilson fermions, W_8 , can be extracted from lattice spectra of the Wilson Dirac operator in the ϵ -regime.

The problem can also be reformulated in terms of a new chiral Random Matrix Theory that describes spectral correlation functions of the Wilson Dirac operator in the appropriate scaling regime. These results open a new domain of Random Matrix Theory where chiral ensembles merge with Wigner-Dyson ensembles. Essen-

tial to this study is an analysis of the gap of the Wilson Dirac operator at finite mass. Lattice QCD simulations depend crucially on control of this gap and its variation as a function of the lattice spacing. As we have stressed, our results are not only important for understanding the finite lattice spacing effects of Wilson fermions near the chiral limit, but may have interesting applications to tail states in condensed matter systems.

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